The Use of Quantum Cascade Lasers for the Detection of Hazardous Materials

U. Willer*a,b, M. Mordmüellera, and W. Schadea,b,c

aClausthal University of Technology, Institute for Energy Research and Physical Technology, Am Stollen 19B, 38640 Goslar, Germany
bEnergy Research Center of Lower Saxony, Am Stollen 19B, 38640 Goslar, Germany
cFraunhofer Heinrich Hertz Institute, Am Stollen 19B, 38640 Goslar, Germany

BIOGRAPHY

Ulrike Willer received her diploma degree in physics from Christian-Albrechts University Kiel, Germany and her doctoral degree from Clausthal University of Technology, Germany. Since 2001 she is member of scientific staff at Clausthal University of Technology. She spent research stays at LBNL, Berkeley, CA and Rice University, Houston, TX.

She has longstanding experience with mid-infrared spectroscopy starting from difference frequency generation with diode lasers up to the deployment of quantum cascade lasers. Her research interests include mid-infrared and photoacoustic spectroscopy, especially quartz enhanced photoacoustic spectroscopy, evanescent-field sensing and the development of sensor devices

TECHNICAL ABSTRACT

Mid-infrared spectroscopy possesses many advantages as sensing technology for hazardous materials: As an optical method, it is capable of online and in-situ measurements and does not rely on sample preparation. Due to the fact, that most molecules possess distinct absorption features within the so called fingerprint region, selective detection is possible if the absorption lines are carefully chosen off site those of possible interferents. Furthermore, the line strength of mid-infrared absorption lines is enhanced as compared to the near-infrared, thus an increased sensitivity can be achieved. These advantages have prompted increasing use in sensing applications.

However, especially for hazardous substances some challenges remain. Obviously, the operator of the sensor device should not be posed at risk, thus a remote and if possible standoff detection is requested. This approach is discussed for the detection of nitric oxide. A DFB QCL is aimed at the probing volume in some distance (20m) and the reflected and backscattered radiation is collected with a telescope (diameter = 40cm) and aligned onto a detector. Figure 1 shows a measurement for the probing volume (cell with 1000ppm NO at p=400mbar) being in 20m distance, and for comparison a simulation using data from the Hitran database. The deducted limit of detection is approximately 90ppm.

The second application of QCLs that will be discussed is the detection of explosives, which is associated with several challenges: (1) most explosives are molecules that are composed of multiple atoms leading to a broad absorption spectrum with bands rather than distinct absorption lines, (2) most explosives possess a very low vapor pressure and are present in low concentrations only, (3) often, they are present as residues only since their presence is tried to being concealed, and (4) there are a vast number of energetic materials and constantly new substances are created that might not be distinguishable from background substances with existing measurement routines.

To identify a hazardous substance, it is therefore necessary to measure at predefined spectral positions to address the specified substance and to exclude possible interferents from consideration. Ideal laser sources for this purpose are broadly tunable external cavity quantum cascade lasers (EC-QCLs). Since the spectral features are broad, pulsed QCLs are readily applicable. One of the substances of interest is triacetone triperoxide (TATP) since it is hard to detect with the commonly used state of the art methods. Figure 2 shows in the upper panel a measurement of TATP with an EC-QCL and a compact multipath cell with optical pathlength of l=1.56m and in the lower panel a FTIR spectrum for comparison. The absorption bands are clearly visible. The measurement shows a considerable noise floor and also fluctuations, especially in the here not shown lower wavelength region. However, it has to be noted that the data were not processed and no noise suppression techniques like lock-in detection have been used so far.
Further examples of the deployment of QCLs for the detection of hazardous substances as e.g. nitrous fumes, methane and explosives will be discussed.

**Keywords:** Mid-infrared spectroscopy, standoff, NO, explosives, TATP, energetic material, EC-QCL